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AB INITIO AND *AB EXITU* NO CORE SHELL MODEL

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We outline two complementary approaches based on the no core shell model (NCSM) and present recent results. In the *ab initio* approach, nuclear properties are evaluated with two-nucleon (NN) and three-nucleon interactions (TNI) derived within effective field theory (EFT) based on chiral perturbation theory (ChPT). Fitting two available parameters of the TNI generates good descriptions of light nuclei. In a second effort, an *ab exitu* approach, results are obtained with a realistic NN interaction derived by inverse scattering theory with off-shell properties tuned to fit light nuclei. Both approaches produce good results for observables sensitive to spin-orbit properties.

Keywords: Light nuclear properties; Chiral effective field theory; Inverse scattering potentials, Many-body theory.

1. Introduction

Recent advances in microscopic many-body methods have opened new paths for investigating both the strong interaction itself as well as the many facets of nuclear phenomena evident in light nuclei. Once the *ab initio* no core shell model (NCSM) was introduced and shown to be reasonably convergent,[1] opportunities emerged for precision testing of the properties of the strong interaction in the nuclear medium. Our focus in this presentation will be on two recent and complementary efforts to determine important features of the strong interaction through the resulting properties of nuclei in the p-shell. Selected observables are especially sensitive to the three-nucleon interaction (TNI) and to the off-shell properties of the NN interaction.

In the first approach,[2] we invoke the power of chiral perturbation theory (ChPT)[3] that provides a promising bridge with the accepted relativistic quantum field theory of the strong interactions, QCD. Beginning with the pionic or the nucleon-pion system[4] one works with systems of increasing nucleon number.[5–7] One makes use of the explicit and spontaneous breaking of chiral symmetry to systematically expand the strong interaction in terms of a characteristic small momentum of a few hundred MeV/c divided by the chiral symmetry breaking scale of about 1 GeV/c. Results should be trustworthy for observables dominated by momentum scales below this characteristic small momentum and thus, we expect the derived interactions to be valid for low-energy nuclear properties.

We adopt the potentials of ChPT at the orders presently available, N3LO for the NN interaction[8] and N2LO for the TNI[9] . The ChPT expansion divides the interactions into perturbative and non-perturbative elements. The latter are represented by a finite set of constants at each order of perturbation theory that are not presently calculable from QCD but can be fixed by measured properties of nuclei provided the many-body methods are sufficiently accurate. Once the non-perturbative constants are determined, the resulting Hamiltonian predicts, in principle, all other nuclear properties, including those of heavier nuclei with no residual freedom. We refer to this first effort as an application of the *ab initio* NCSM since the NN interaction is completely fixed by properties of the two-body system. Important components of TNI and higher-body interactions are also fixed by the ingredients of the NN terms. Only residual non-perturbatve chiral TNI couplings are fixed, as necessary, by the properties of nuclei beyond $A = 2$. Eventually, independent methods such as lattice QCD should fix all these parameters and complete the *ab initio* NCSM so the need for fitting would be eliminated.

In the second approach[10] the NN interaction is taken as a finite rank separable form in an oscillator representation for each partial wave. The coefficients are determined, to the extent possible, by inverse scattering techniques[11] using the available NN data. Subsequently, one investigates off-shell freedoms with phase-shift equivalent unitary transformations to tune the interaction to fit the properties of light nuclei. By fitting the ^3He and ^{16}O binding energies and the ^6Li low-lying spectra we obtain the interaction "JISP16", which represents "J-matrix Inverse Scattering Potential tuned up to ^{16}O". We achieve soft interactions with this approach that describe all the data conventionally fit by realistic NN interactions and provide good fits to light nuclear properties.[10] We consider this as a phenomenological approach designed to explore regions of NN interactions that are not yet explored by other methods. We hope that the phase-shift equivalent transformation methods that prove successful in this *ab exitu* NCSM will be useful for minimizing higher-body forces in other approaches. This would be helpful for gaining access to heavier nuclei within the NCSM.

In many instances we find the results of both approaches to be similar and we cite the example of ^{10}B in the present work.

2. No core shell model (NCSM)

The NCSM casts the diagonalization of the infinite dimensional many-body Hamiltonian matrix as a finite matrix in a harmonic oscillator (HO) basis with an equivalent "effective Hamitonian" derived from the original Hamiltonian.[1] The finite matrix is defined by N_{max}, the maximum number of oscillator quanta shared by all nucleons above the lowest configuration. We solve for the effective Hamiltonian by approximating it as either a 3-body interaction[12] based on our chosen NN+TNI from ChPT (our *ab initio* application) or a 2-body interaction based on JISP16 (our *ab exitu* application). With these "cluster approximations", convergence is guaranteed with increasing N_{max} or with increased cluster size at fixed N_{max}.[1]

The NCSM is the only approach currently available to solve the resulting many-body Schrödinger equation for mid-p-shell nuclei while preserving all symmetries when the interactions are non-local, a feature of all the interactions employed in this work.

3. *Ab initio* NCSM with interactions from ChPT

In order to motivate the inclusion of the TNI, we begin by showing, in Fig. 1, the natural parity excitation spectra of ^{10}B with the ChPT N3LO NN

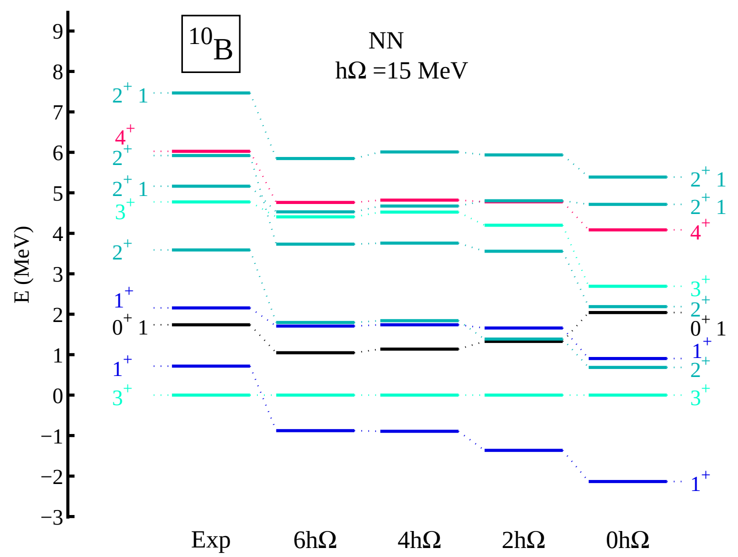

Fig. 1. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state. The NCSM results are obtained with the chiral N3LO potential[8] at an oscillator energy, $\hbar\Omega = 15\ MeV$ as a function of $N_{max}\hbar\Omega$, indicated at the bottom of each spectrum. Note the reasonable convergence as one proceeds up to $N_{max} = 6$ where the dependence on $\hbar\Omega$ (not shown here) is found to be weak.

interaction alone (excluding TNI), using our 3-body cluster renormalization to the finite basis specified by N_{max}. The figure displays results for basis spaces from $N_{max} = 0 - 6$. We note the now-accepted defect with conventional realistic NN interactions: theory and experiment differ by an inversion of the two lowest levels. In addition, the theory spectrum is somewhat compressed relative to experiment. Over the past few years, these deficiencies, as well as others in mid-p-shell nuclei, such as binding energies, spectral properties and electromagnetic transition rates, have been ascribed to the need for TNI's. In terms of physics, the inadequacy of the realistic NN interactions appears as insufficient spin-orbit splitting in the mean field generated by those interactions, though the mean field itself is not calculated directly. We summarize here the role of the TNI and the role of off-shell modified NN interactions in correcting this inadequacy.

We define the two non-perturbative coupling constants of the TNI, not fixed by 2-body data, as C_D (C_E), the strength of the $N - \pi - NN$ (TNI)

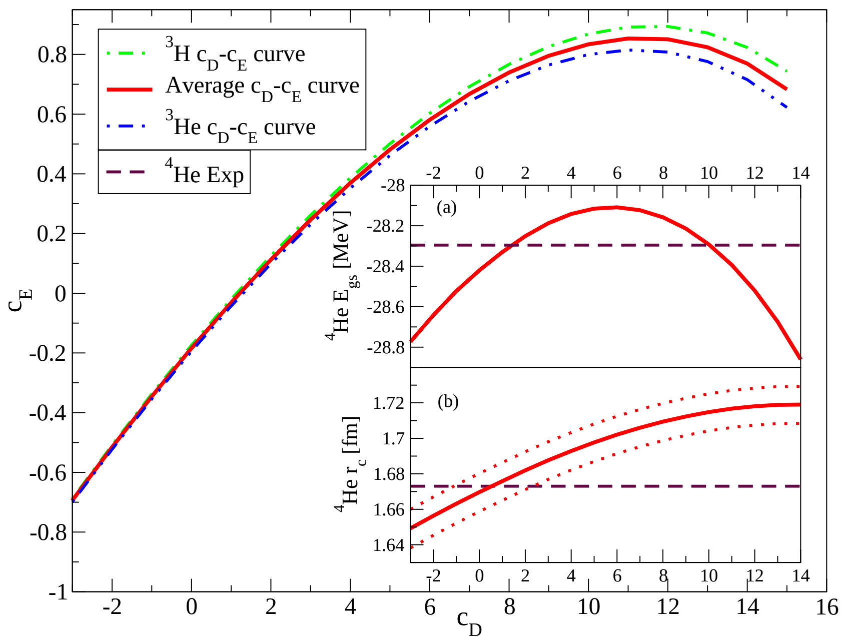

Fig. 2. Relations between C_D and C_E for which the binding energy of ^{3}H (8.482 MeV) and ^{3}He (7.718 MeV) are reproduced. (a) ^{4}He binding energy along the averaged curve. The experimental ^{4}He binding energy (28.296 MeV) defines two points of intersection using the averaged $A = 3$ $C_D - C_E$ curve. (b) ^{4}He charge radius. Dotted lines represent the spread in r_c due to uncertainties in the proton charge radius.

contact term. Fig. 2 shows the trajectories of these two parameters as determined from fitting the binding energies of the $A = 3$ & 4 systems as well as the average of the two trajectories. Our approach is similar to the one used in a detailed investigation[13] of ^7Li. The ^4He results use the average of the $A = 3$ fits and the inset shows two crossing points where the ^4He binding is reproduced. Note the expanded scale. The second inset (b) depicts the corresponding rms charge radius of ^4He.

Our results on the radii of the $A = 3$ systems are in good agreement with experiment as well. While the uncertainties in the ^3H and ^3He charge radii obscure the differences between the intersection points, the ^4He charge radius (inset (b) of Fig. 2) indicates a preference for $C_D \sim 0$ with a broad span of reasonable results around it. This led us to investigate observables in the mass 11-13 range where we find good results $C_D \sim -1$.[2]

An example of the improvement obtained with the TNI of ChPT ($C_D = -1$ on average $A = 3$ curve) is shown in Fig. 3 as compared/contrasted with

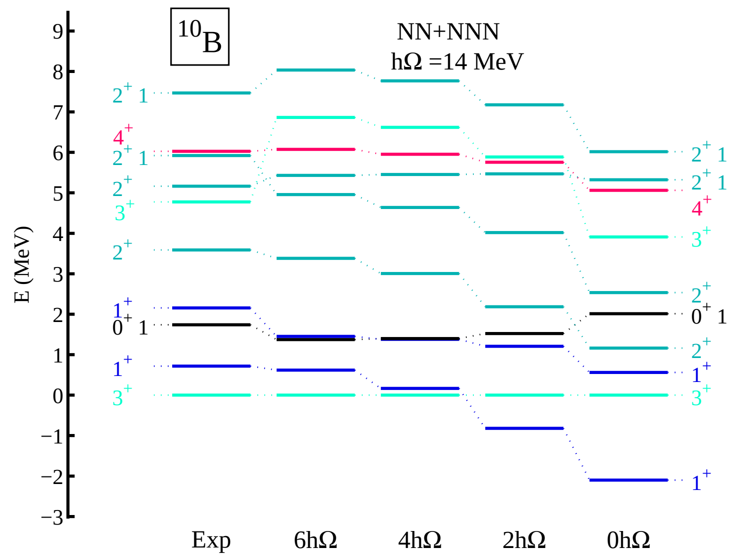

Fig. 3. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state. The NCSM results are obtained with the chiral N3LO potential[8] at an oscillator energy, $\hbar\Omega = 14\ MeV$ as a function of N_{max} indicated at the bottom of each spectrum. Note the reasonable convergence again as one proceeds up to $N_{max} = 6$

Fig. 1. The correct level ordering is now obtained and the spectrum is more spread out in closer agreement with experiment. In addition, the binding energy shifts towards agreement with experiment as seen below in Table 1. Refinements in our NCSM techniques will soon allow us to obtain the spectrum at $N_{max} = 8$ to extend the convergence trends for Figs. 1 and 3.

4. *Ab exitu* NCSM with interaction from inverse scattering

Turning to a sample of results with the *ab exitu* NCSM we present in Fig. 4 the binding energies of stable p-shell nuclei relative to experiment using the JISP16 interaction. Both bare and effective interaction results are presented as well as some initial extrapolations to the infinite basis limit.[14] The bare interaction results are strict upper bounds to the exact ground state energy so the bare curves will drop as the basis space is increased (direction of increased binding in the theory). The effective interaction results do not follow a variational principle. The results show a tendency to underbind nuclei in mid-p-shell and to overbind at the upper end. Results in larger

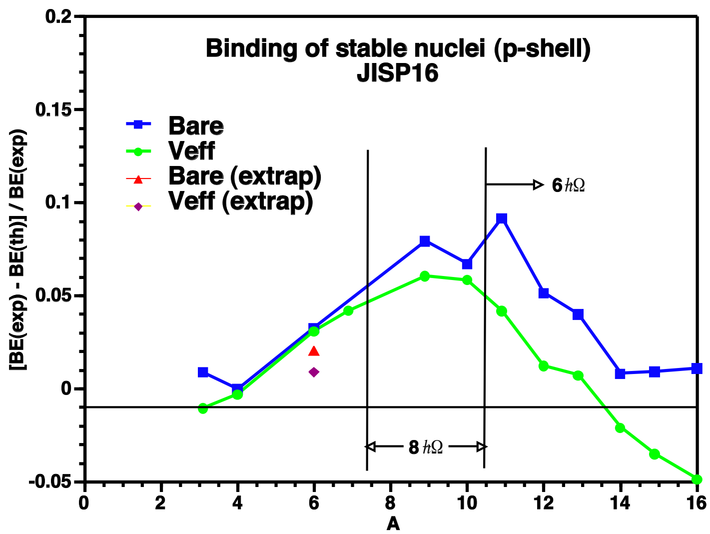

Fig. 4. Fractional difference between theory and experiment for the binding energies of stable p-shell nuclei. The results are quoted with the specified N_{max} values and with both the bare and effective JISP16 interactions. The effective interactions are evaluated at the 2-body cluster level. The oscillator energy, $\hbar\Omega$ is taken, in each case, to be the value at which an extremum in the binding energy occurs.

basis spaces will help clarify these trends.

Towards this goal, we present in Fig. 5 initial results for the ground state energy of ^{12}C in a larger $N_{max} = 8$ basis space using the bare JISP16 interaction and compare with the results obtained in smaller basis spaces. While the convergence trend is encouraging, we note that JISP16 seems on a path to produce modest overbinding. More analyses are in progress to obtain an extropolated ground state energy and its uncertainty.[14]

5. Concluding remarks

Table 1 contains selected experimental and theoretical results for ^{10}B. The binding energy and rms deviation between the experimental and theoretical excitation energies improve substantially with the inclusion of TNI. The JISP16 results lie intermediate to the N3LO and N3LO+TNI interaction results. Other observables are in reasonable accord with experiment considering that (1) we use bare electromagnetic operators, and (2) moments and transition rates are expected to be more sensitive to enlarging the basis

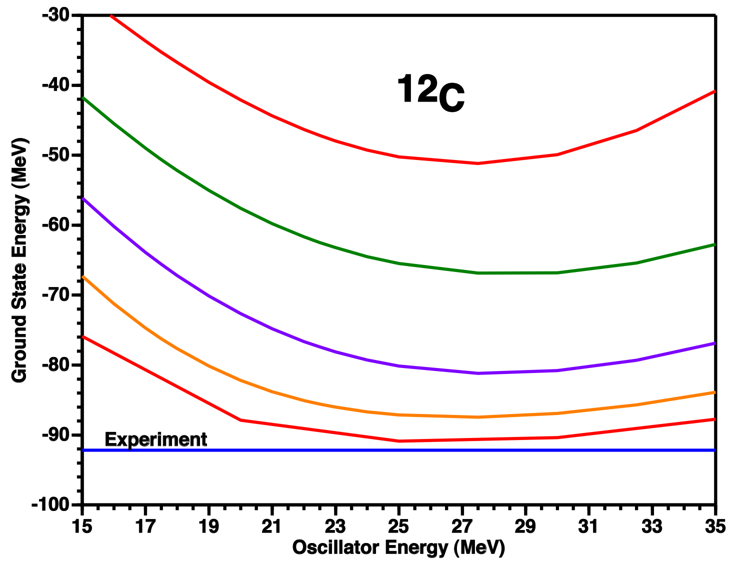

Fig. 5. Ground state energy for ^{12}C as a function of the oscillator energy, $\hbar\Omega$, for $N_{max} = 0 - 8$ for the bare JISP16 interaction. The $N_{max} = 8$ curve is closest to experiment and each curve above it corresponds to decrements by two units in N_{max}.

spaces as we plan to do. The JISP16 results employ partial waves, $J \leq 3$.

These results required substantial computer resources. The $N_{max} = 6$ spectrum shown in Fig. 3 and a set of additional experimental observables, takes an hour on 3500 processors on the LLNL-Thunder machine. Our largest run that is reported here, the ^{12}C with JISP16 in the $N_{max} = 8$ basis ($dimension = 6 \times 10^8$) took 2.3 hours on 15,400 processors (33,350 cpu hours) at the ORNL Jaguar facility. All runs produce the lowest 15 converged eigenvectors and a suite of observables (rms radii, electromagnetic moments and transitition rates, electroweak transition rates, etc.).

We demonstrated here that TNI's make substantial contributions to improving the spectra and other observables. In addition, phase-equivalent transformations of an interaction obtained from inverse scattering, JISP16, produces appealing fits to light nuclear properties. However, there is considerable room for further improvement in both approaches. Our leading suggestions include: (1) extend the TNI's to the order consistent with the NN interaction, N3LO; (2) extend the basis spaces to higher N_{max} values to

Table 1. Properties of ^{10}B from experiment and theory. E2 transitions are in e^2 fm^4 and M1 transitions are in μ_N^2. The rms deviations of excited state energies are quoted for the lowest 9 states whose spin–parity assignments are well established and that are known to be dominated by $0\hbar\Omega$ configurations. Results are obtained in the basis spaces $N_{\max} = 6(8)$ with $\hbar\Omega = 14$ MeV for the ChPT (JISP16 up through $J = 3$ partial waves) interaction. In the $N3LO+TNI$ column we show selected sensitivity to changing C_D by ± 1. "N/A" indicates a result yet to be calculated. The experimental values are from Ref.[15,16]

Nucleus/property	Exp	$N3LO$ $+TNI$	$N3LO$	JISP16
$^{10}B:\ \lvert E(3^+,0)\rvert$ [MeV]	64.751	64.78	56.11	59.715
r_p [fm]	2.30(12)	2.197	2.256	2.204
$Q(3_1^+,0)$ [e fm^2]	+8.472(56)	+6.327	+6.803	6.704
$\mu(3_1^+0)$ [μ_N]	+1.801	+1.837	+1.853	N/A
$E_{\rm x}(3_1^+0)$ [MeV]	0.0	0.0	0.0	0.0
$E_{\rm x}(1_1^+0)$ [MeV]	0.718	0.523	-1.128	0.185
$E_{\rm x}(0_1^+1)$ [MeV]	1.740	1.279	0.913	1.023
$E_{\rm x}(1_2^+0)$ [MeV]	2.154	1.432	1.643	2.215
$E_{\rm x}(2_1^+0)$ [MeV]	3.587	3.178	1.643	3.424
$E_{\rm x}(3_2^+0)$ [MeV]	4.774	6.729	4.193	5.790
$E_{\rm x}(2_1^+1)$ [MeV]	5.164	5.315	4.419	4.856
$E_{\rm x}(2_2^+0)$ [MeV]	5.92	4.835	3.555	5.195
$E_{\rm x}(4_1^+0)$ [MeV]	6.025	5.960	4.790	5.775
$E_{\rm x}(2_2^+1)$ [MeV]	7.478	7.823	5.565	7.311
$rms(Exp-Th)$ [MeV]	-	0.823	1.482	0.535
B(E2;$1_1^+0 \to 3_1^+0$)	4.13(6)	3.05(62)	4.380	3.732
B(E2;$1_2^+0 \to 3_1^+0$)	1.71(0.26)	0.50(50)	0.082	0.578
B(M1;$2_1^+0 \to 3_1^+0$)	0.0015(3)	0.0000	N/A	0.0012
B(M1;$2_1^+1 \to 3_1^+0$)	0.041(4)	0.216	N/A	0.125
B(M1;$2_2^+0 \to 3_1^+0$)	0.050(12)	0.053	N/A	0.056
B(M1;$4_1^+0 \to 3_1^+0$)	0.043(7)	0.002	N/A	N/A
B(M1;$2_2^+1 \to 3_1^+0$)	-	4.020	N/A	4.148
B(GT;$3_1^+0 \to 2_1^+1$)	0.083(3)	0.07(1)	0.102	0.040
B(GT;$3_1^+0 \to 2_2^+1$)	0.95(13)	1.22(2)	1.487	1.241

further improve convergence; (3) examine sensitivity of TNI's to the choice of regulator; and (4) include four-nucleon interactions at a consistent order of ChPT. In addition, further exploration of the phase-shift equivalent transformations appears warranted.

Our overall conclusion is that these results support a full program of deriving the NN interaction and its mulit-nucleon partners in the consistent approach provided by chiral effective field theory. It is straightforward, but challenging, to extend this research thrust in the directions indicated. However, the favorable results to date and the need for addressing fundamental symmetries of strongly interacting systems with enhanced predictive power, firmly motivates this path.

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